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Ionic structure in electrolyte confined by dielectric interfaces

YUFEI JING, Northwestern University, VIKRAM JADHAO, Johns Hopkins University, JOS W. ZWANIKKEN, University of Massachusetts, Lowell, MONICA OLVERA DE LA CRUZ, Northwestern University — The behavior of ions in liquids confined between macromolecules determines the outcome of many nanoscale assembly processes in synthetic and biological materials. To model these systems, both the macromolecules and the surrounding solvent are treated as continuous media characterized with different dielectric permittivities. As the macromolecule-liquid boundary is modeled as a dielectric interface, an important quantity of interest is the ionic structure in a liquid confined between two such interfaces. We compute the ionic structure in a model system of electrolyte confined by two planar dielectric interfaces using molecular dynamics simulations and liquid state theory. We give a comprehensive description of the effects of high electrolyte concentrations, multivalent ions, dielectric contrasts, and external electric field on the ionic distributions. We observe novel features in ionic structure near polarizable/unpolarizable macromolecules which is attributed to the competition between electrostatic and steric (entropic) interactions. We argue that the combined effect of ionic correlations and inhomogeneous dielectric permittivity significantly changes the character of the effective interaction between the two macromolecules.

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